

Goals

(1) Develop theories of properties of solids

- Crystal structure - (defects, glasses)
 how far apart are nuclei? pattern to arrangement?
 vibrations - conduction of sound/heat

focus on \rightarrow
 nuclei
 (ultimately then
 "glue" is e^-)

structural properties - bulk, shear moduli

- "electronic structure"

$$\kappa = -V \frac{dP}{dV} \quad dV = -\frac{1}{\kappa} V dP$$

metal, insulator, semiconductor

- optical properties - color, transparency

response to general EM field

$$\begin{aligned} \text{Ideal gas } V &= \frac{NkT}{P} \\ dV &= -\frac{NkT}{P^2} dP \\ &= -\frac{1}{P} V dP \end{aligned} \quad \left[\frac{dT}{T} = 0 \right]$$

- Exotic properties

can depend on ω

magnetism

superconductivity

(2) Understand experiments which reveal properties

- neutron scattering, x-ray scattering, STM

- conductivity, Hall Effect

- de Haas van Alphen
 Josephson effect
 nuclear magnetic resonance

(3) Long standing realization that symmetry plays a key role but recently this has been explored in some very new + exciting ways

(1) \leftrightarrow (2) Crucial to develop theory of response of solid to external probe (experiment)

$$\chi = M/B \quad \text{DIPOLAR}$$

$$\sigma = J/E$$

$$M(q, \omega) = \chi(q, \omega) B(q, \omega)$$

$$\sigma(q, \omega)$$

Solid State Physics

Along with astronomy, the oldest subfield of physics
ages of mankind cm names!

Pre-scientific times: stones, bronzes, iron, jewelry

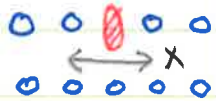
→ A lot of empirical knowledge but prior
to end of 19th century almost no understanding

Mix carbon
in iron
→ steel.

prevents
planes
of iron atoms
fr sliding
past each
other

Crystals: periodic structure of atoms
common notion in mineralogy
first proven by x-rays 1912

Despite long history continual history of new discoveries
both experiment and theory



Current "hot topics"

insulators in bulk, conduct at surface

topological insulators

eigenstate thermalization hypothesis

→ quantum quenches

Moiré patterns in bilayer graphene

quantum entanglement

To what extent is a single
eigenstate of \hat{H}
with a particular energy E
representative of
behavior of system at
temperature T giving
that same E on average?

t evolution
after
sudden
change in T
→ after sudden
change in
parameter
in \hat{H}

Girvin Yang Table of Contents

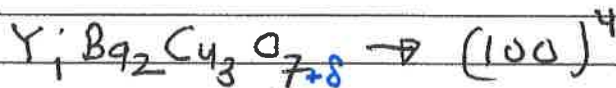
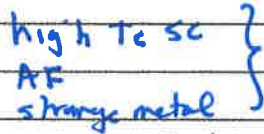
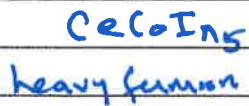
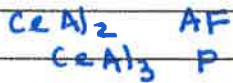
Find 140 Notes.
and problems

- 1) overview of CM physics
- 2) spatial structure
- 3) Lattices and Symmetries
- 4) Neutron scattering
- 5) Dynamics of Lattice Vibrations
- 6) Quantum Theory of Harmonic Crystal
- 7) Electronic structure of crystals ← {tight binding models}
- 8) Semiclassical transport theory
- 9) semiconductors
- 10) Nonlocal transport in mesoscopic systems
- 11) Anderson localization
- 12) Integer Quantum Hall Effect
- 13) Topology and Berry phase
- 14) Topological Insulators and Metals
- 15) Interacting Electrons
- 16) Fractional Quantum Hall effect
- 17) Magnetism
- 18) Bose Einstein Condensation
- 19) Superconductivity: phenomena and phenomenological theory
- 20) Superconductivity: Microscopic Theory

Fin.
Introduction

A vast, challenging field [Amazing we can do anything!]

(1) 100 or so elements in periodic table



Makes CMP
different from HEP,
NP, even cosmology
↑ fewer ways to
"combine things"

(2) Hydrogen atom 1 proton + 1 electron

Laguerre polynomials, Spherical Harmonics...

in solving Schroedinger Eqn.

Now 10^{23} e^- and nuclei

(3) Not only different "ingredients" (1)

but different dimensionalities

$d=0$ nanodots

$d=1$ nanotubes

$d=2$ magnetic multilayer

$d=3$ bulk

(4) And different "environments"

low $T \rightarrow$ superconductivity

high $P \rightarrow$ { magnet \rightarrow nonmagnetic
insulator \rightarrow metal
lattice structure changes

Intro

Matter surrounding us 10^{23} atoms/molecules
 of size 10^{-10} m $\sim 1 \text{ \AA}$.

Gas: interparticle spacing $\gg 1 \text{ \AA}$

-
- * particles interact weakly
 - * particles maintain "integrity"

Liquids/Solids interparticle spacing $\sim 1 \text{ \AA}$

be a bit
 careful about
 link between
 high density
 and strong
 interaction

fining
 characteristic
 of CM system

- * strong interactions
- * e^- can become detached from individual atoms

↳ properties of CM system differ markedly
 from those of atomic constituents

$k_B = 1.38 \cdot 10^{-23}$

$T = 300^\circ \text{K}$

$k_B T \sim .0235 \text{ eV}$

whereas for an atom energy $\sim 13.6 \text{ eV}$



Because $k_B T \ll E_n$ changing T is
 not going to affect properties of an individual H
 atom or H_2 molecule.

I1A

SKIP.

Gas

$$PV = Nk_B T$$

$$d^3 = \frac{V}{N} = \frac{k_B T}{P} = \frac{1.38 \cdot 10^{-23} \cdot 300}{10^5} \sim 4 \cdot 10^{-26}$$

$$1 \text{ atm} = 1.01 \cdot 10^5 \text{ N/m}^2$$

$$d = (40 \cdot 10^{-27})^{1/3} \sim 3.4 \cdot 10^{-9} = 34 \text{ \AA}$$

Solid / liquid

$$\rho(\text{H}_2\text{O}) = 1 \text{ g/cm}^3$$

$$\text{molecule of H}_2\text{O} = 18 (1.67 \cdot 10^{-27}) \text{ g}$$

$$\frac{N}{V} = \frac{1}{18(1.67 \cdot 10^{-27})} \frac{1}{\text{cm}^3}$$

$$= \frac{1}{3 \cdot 10^{-26}} \frac{1}{(10^{-2} \text{ m})^3} = \frac{1}{3 \cdot 10^{-32}} \frac{1}{\text{m}^3}$$

$$d^3 = \frac{V}{N} = 3 \cdot 10^{-32} = .03 \cdot 10^{-30}$$

$$d \sim .31 \cdot 10^{-10} \text{ m} = .31 \text{ \AA}$$

12.

The fact that CM form solid structures from liquids, become magnetic, become superconducting as T is varied \rightarrow low energy excitations must emerge from the close proximity of atoms.

A big part of CM is the determination of those low energy excitations

I 3.

TOPIC # 1

Classifying Solids

* By chemical constituents

Elemental Solids ~ 100 \leftarrow what limits

2 Elements NaCl, MgB₂ \leftarrow pretty high T_c SC

3 Elements CaV₄O₉ \leftarrow "spin liquid"

CeCoIn₅ \leftarrow heavy fermion

4 Elements La_{2-x}Sr_xCuO₄ high Temperature (cuprate) SC

CeAl₂ magnetic
CeAl₃ nonmagnetic

Iron pnictide SC

\swarrow non-oxy pnictide
 FeSe
 Ba_{0.6}K_{0.4}Fe₂As₂

\downarrow oxy pnictide
 NdFeAsO_{0.89}F_{0.11}
 \uparrow T_c = 52°K

topological insulators CdTe/HgTe/CdTe 2D
Bi₂Se₃ 3D

graphene C  pattern : "Dirac Fermions"

Should be evident why CM is such a rich field
100 elements in groups of eg 4 $\rightarrow 10^8$ materials

I 4.

* Classify by Atomic positions

periodic array of nuclear positions

(random: liquid/glass)

↑ everything solidifies if T is low enough except He

* Classify by properties

ability to transport charge

{ a) metal, insulator, semiconductor, superconductor

magnetic behavior

b) paramagnet, diamagnet, ferromagnet, antiferromagnet

↗
(?) Name some MnO , FeO , CoO
transition metal oxides

parent compounds of
cuprate SC



CuO_2 planes

* Classify by Symmetries

symmetry: a transformation leaving Hamiltonian invariant

specific phases might break symmetry

Eg $\vec{r}_e \rightarrow \vec{r}_e + \vec{c}$ translation leaves \hat{H} unchanged
 (pairwise potentials $V(\vec{r}_e - \vec{r}_n)$)

But in a perfect crystal atoms are in particular locations, breaking T

Ferromagnets & Antiferromagnets break spin rotation symmetry and time reversal symmetry
 (AF also break translation symmetry)

order parameter: measurable physical quantity which transforms nontrivially under a symmetry operation which leaves H invariant.

What is order parameter of a superfluid or superconductor?

I 6.

Topological phases: same symmetry but distinct nevertheless. Eg band insulator & metal.

Distinction is instead topological: the number of fermi surface sheets.

Theory: complete description: solve Many particle Sch. Eqn.

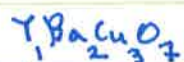
Impossible (even for He!, just 2 electrons)

key idea to move forward: focus on the low energy excitations (and possibly create models which incorporate discarding the excitations which are frozen out).

Already: do not allow nuclei to break (MeV scale)

Cuprates: particles live in widely separated CuO_2 sheets
in fact mostly on Cu atoms

Hint: all cuprates have CuO_2 sheets



square lattice

already gives important ideas about cuprate

physics, eg d-wave SC symmetry

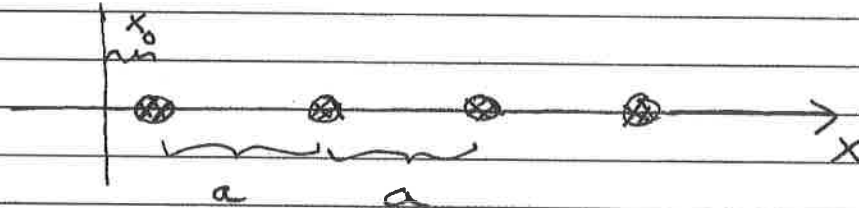
(skip I-3)

project:

I-4

Crystals are periodic arrays of atoms. We will start in low d since easier to draw.

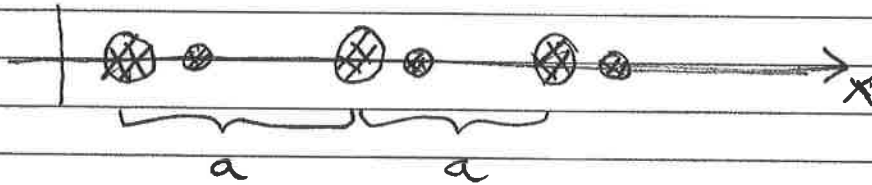
Suppose only one type of atom:





Atoms located at $x = x_0 + na$

might as well choose $x_0 = 0$ for simplicity

If more than one type of atom:



one specifies the separation " a " but also the "basis"

ie the collection of atoms   that repeats

Note the lattice looks the same if you look at set of lattice points $x_0 + n(2a)$ or $x_0 + n(3a)$

but the $x_0 + na$ set is said to be primitive because it has the smallest length (area, volume)

DIVOGA

(skip I-6)

project:

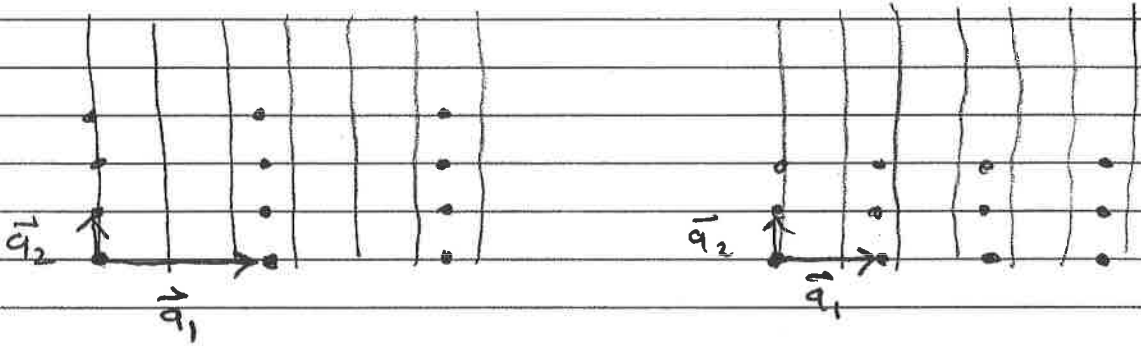
I-7

Natural to ask how many "types" of lattice there are

What do we mean by "type"?

Would you consider lattices with $\vec{a}_1 \perp \vec{a}_2$

and $|\vec{a}_1| = 2.7|\vec{a}_2|$ different from $|\vec{a}_1| = 1.9|\vec{a}_2|$?



$$|\vec{a}_1| = 2.7|\vec{a}_2|$$

$$|\vec{a}_1| = 1.9|\vec{a}_2|$$

If you say "different" then there are clearly an ∞ # of lattices in 2d corresponding to the ∞ # of choices of $|\vec{a}_1|/|\vec{a}_2|$

What else could you do?

Instead base definition of type on symmetry.

Lattice which is invariant under rotation by $\pi/2$ must

be a square lattice $\vec{a}_1 \perp \vec{a}_2$ and $|\vec{a}_1| = |\vec{a}_2|$

"4 fold axis"

same
in sense
that if
you rotate
by π
you get
original
lattice

HW

project:

I-7'

Argument for # lattice types in $d=2$

set scale of length

without loss of generality can choose $\vec{a}_1 = (1, 0)$

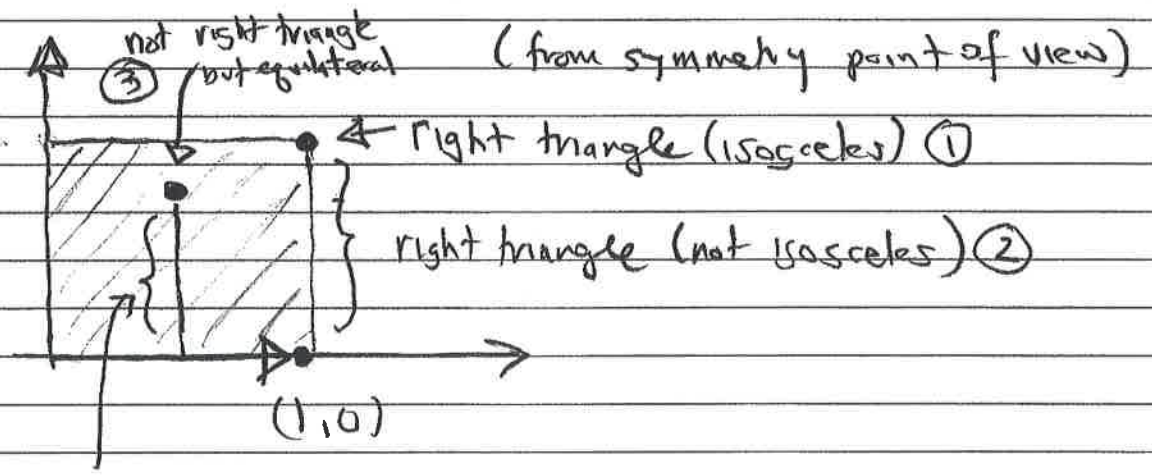
Then also can choose $\vec{a}_2 = (x, y)$ with $y > 0$

$x < 1$



make \vec{a}_1 be the longer of 2 vectors
x component

Now ask: what special (x, y) there are



there is also a right triangle isosceles on this path but equivalent to (1) in symmetry sense

not right triangle, not equilateral but isosceles (4)

(5) anything else "oblique"

CRYSTAL: ATOMIC POSITIONS FORM REGULAR ARRAY

project:

I-5

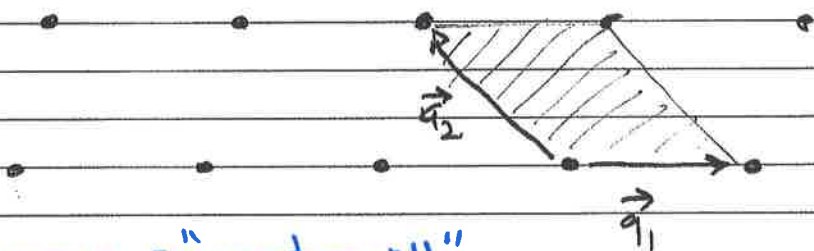
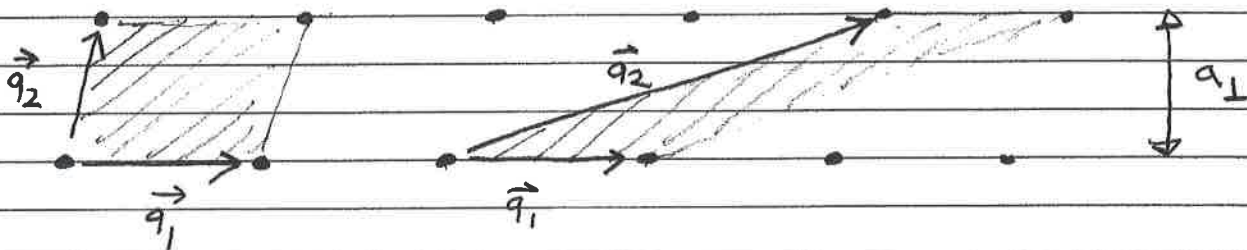
↑
amazing energy bands
of solids same mechanism!

Bravais Lattice:

In 2d need 2 vectors

collection of points

$$\vec{R} = n_1 \hat{a}_1 + n_2 \hat{a}_2 + n_3 \hat{a}_3$$



2D \hat{a}_1, \hat{a}_2 not
collinear

3D $\hat{a}_1, \hat{a}_2, \hat{a}_3$
not coplanar

shaded area is "primitive cell"

There are also many choices of \vec{a}_1, \vec{a}_2 which are primitive

(smallest area). All choices above have same area $|\vec{a}_1 \times \vec{a}_2|$

WHY? $\vec{a}_1 \times \vec{a}_2 = |\vec{a}_1| |\vec{a}_2| \sin \theta_{12}$

and in pictures above $|\vec{a}_2| \sin \theta_{12} = a_{\perp}$ is

same for all choices

Again, lattice will look the same with some choices of

\vec{a}_1 and \vec{a}_2 with bigger $|\vec{a}_1 \times \vec{a}_2|$ but then we will

not call them "primitive"

attaching primitive cell to each point of Bravais
lattice will fill up all space.

DIVOGA

Q:

Volume in 3D
 $\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$

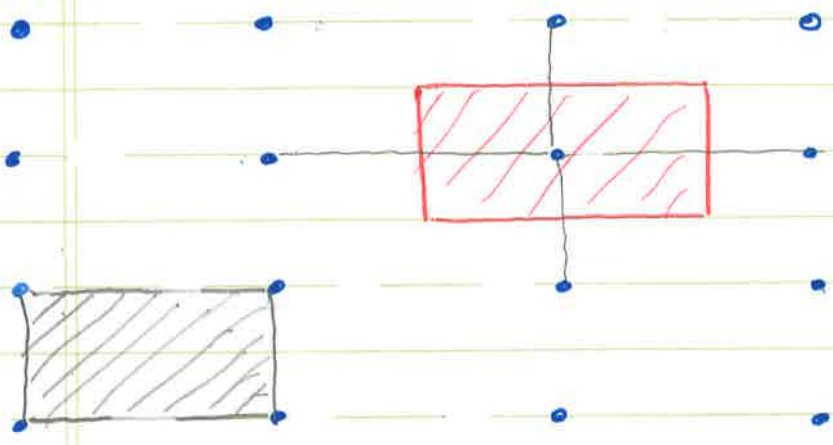
A particular type of primitive cell:

"Wigner-Seitz primitive cell"

region of space closer to a given point

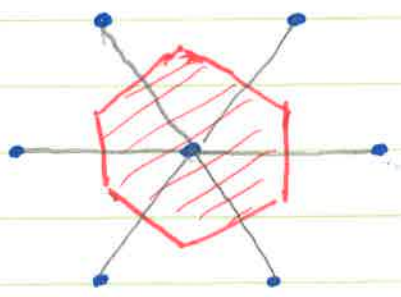
than to any other lattice point

RECTANGULAR



* draw lines to nearest neighbors
* draw bisectors

TRIANGULAR



Popular Lattices

Only Polonium of all elements

Reason: It is too empty!

Simple Cubic

$$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

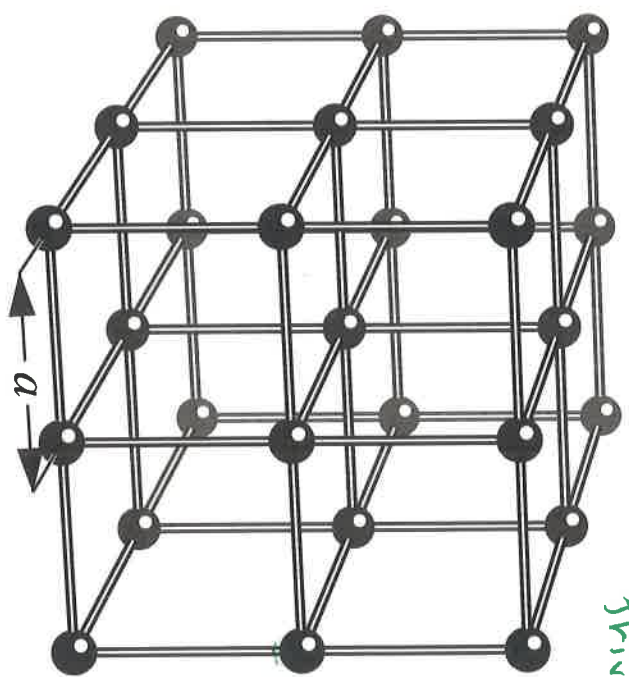
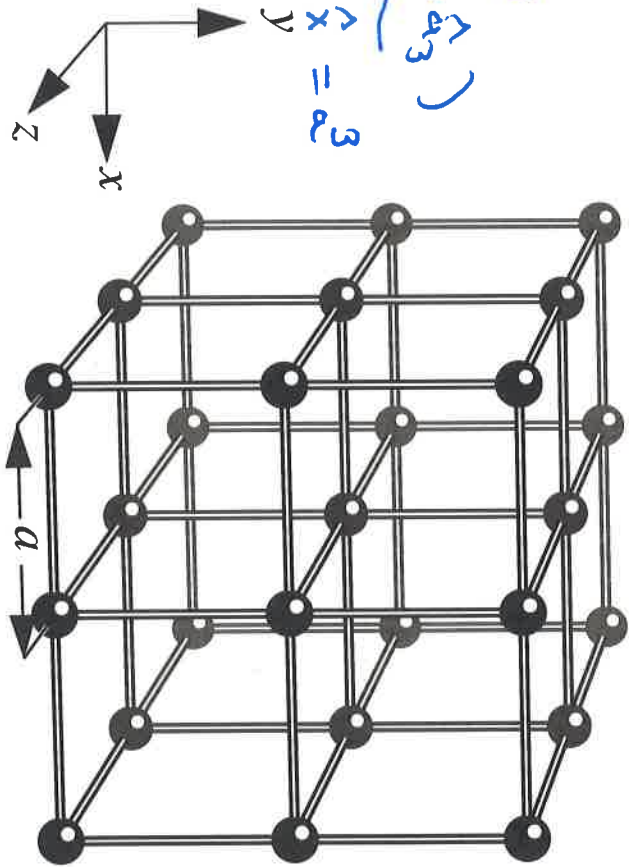
Primitive lattice vectors
 $\vec{a}_1 = a \hat{x}$ $\vec{a}_2 = a \hat{y}$ $\vec{a}_3 = a \hat{z}$

Trivial here

Volume is

$$\hat{a}_1 \cdot (\hat{a}_2 \times \hat{a}_3)$$

$$a \hat{x} \cdot a^2 \hat{x} = a^3$$



To view these crystals in 3-d, install **rasmol**. Using xpdf version 2, one can click on the name above each figure and invoke rasmol automatically. Configure rasmol with a .rasmolrc file

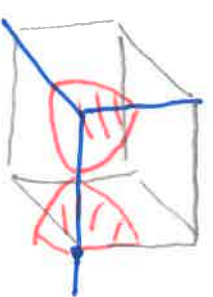
containing

[Packing fraction calculation here](#)

spacefill 100

$$V = a^3$$

$$\text{spheres } 8 \cdot \frac{1}{8} \pi \left(\frac{a}{2}\right)^3$$



wireframe 20

$$= \frac{\pi}{6} a^3$$

$$\text{Packing fraction} = \frac{\pi}{6} = .524$$

Popular Lattices

| | | | |
|----|------|----|----|
| Ba | 5.02 | Li | Ta |
| Cr | 2.88 | Mo | Ta |
| CS | 6.05 | Na | V |
| Fe | 2.87 | Nb | |
| K | 5.23 | Rb | |

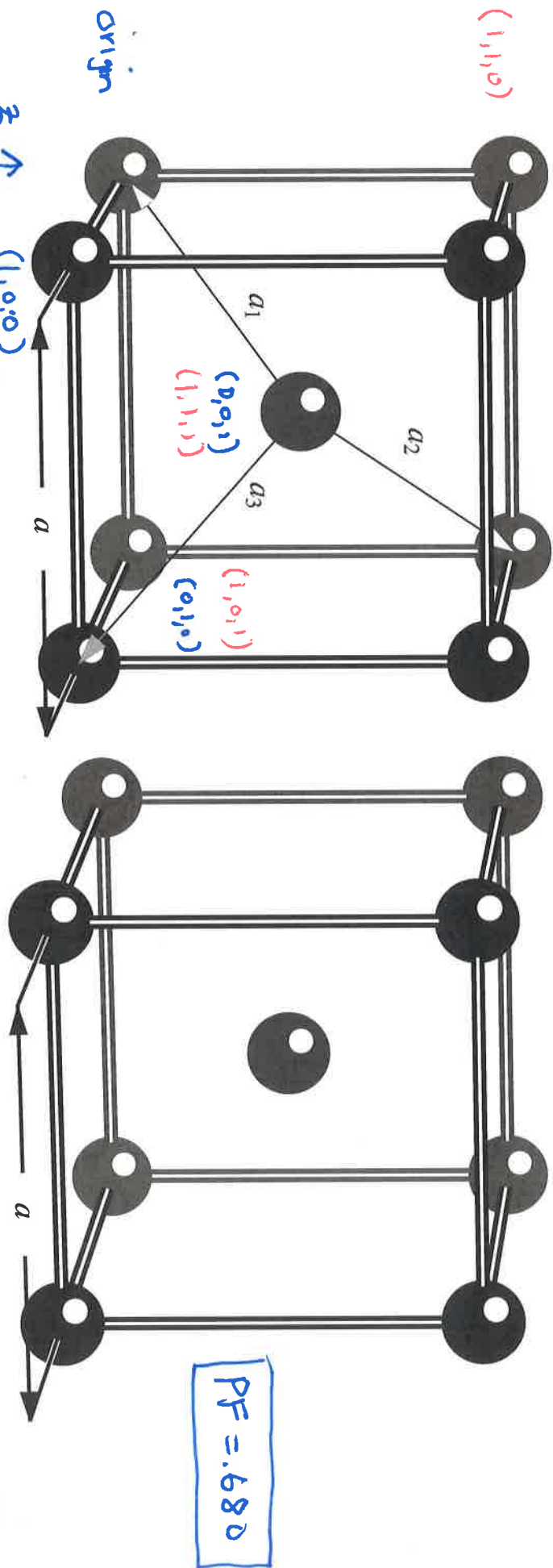
Body Centered Cubic (bcc)

14 elements

$$\begin{aligned} \hat{a}_1 &= a\hat{x} \\ \hat{a}_2 &= a\hat{y} \\ \hat{a}_3 &= \frac{a}{2}(\hat{x} + \hat{y} + \hat{z}) \end{aligned}$$

MORESTWNETRIC

$$\begin{aligned} \vec{a}_1 &= \frac{a}{2}(-\hat{x} + \hat{y} + \hat{z}) \\ \vec{a}_2 &= \frac{a}{2}(\hat{x} - \hat{y} + \hat{z}) \\ \vec{a}_3 &= \frac{a}{2}(\hat{x} + \hat{y} - \hat{z}) \end{aligned}$$



$$\left| \hat{a}_1 \cdot (\hat{a}_2 \times \hat{a}_3) \right| = a^3/8 (2 + 2 + 2) = 3/4 a^3$$

$$a^2/4 \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{vmatrix} = a^2/4 (-2\hat{x} + 2\hat{y} + 2\hat{z})$$

Popular Lattices

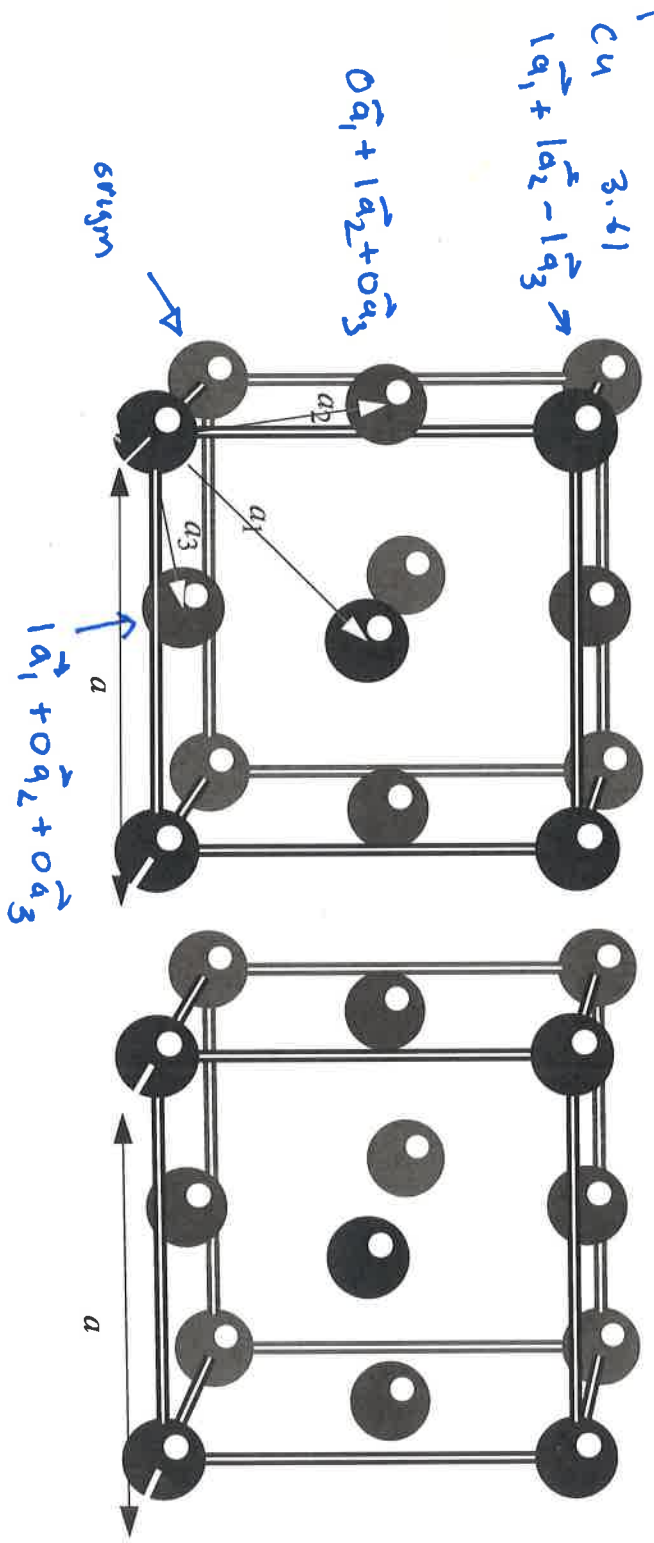
| | | |
|-------------|------|----|
| Ar | 5.26 | In |
| Ag | 4.09 | Kr |
| Al | 4.05 | La |
| Au | 4.08 | Ne |
| Cu | 5.58 | Ni |
| ce | 5.16 | Pb |
| β -Co | 3.55 | Pt |

| | |
|------|---------------------------|
| Pt | Sr |
| 8-Ru | Face Centered Cubic (fcc) |
| Rh | (24 elements) |
| Sc | |
| Th | |
| Xe | |
| Yb | |

$$\vec{a}_1 = \frac{a}{2}(\hat{y} + \hat{z})$$

$$\vec{a}_2 = \frac{a}{2}(\hat{x} + \hat{z})$$

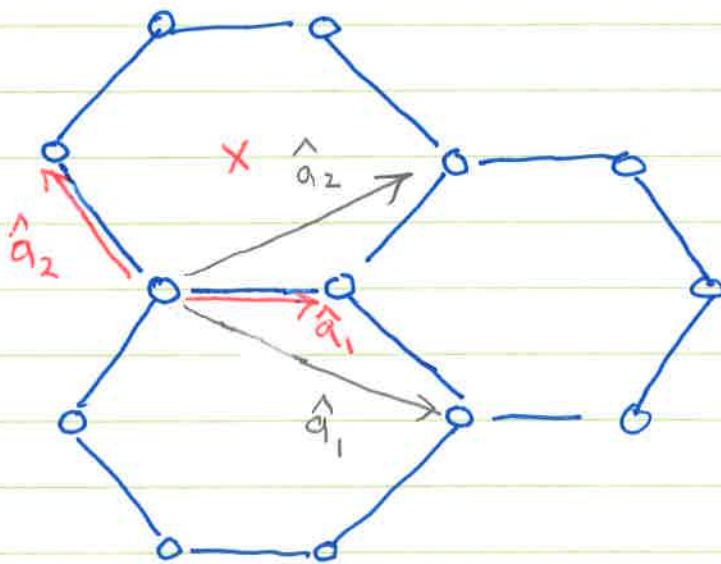
$$\vec{a}_3 = \frac{a}{2}(\hat{x} + \hat{y})$$



$$PF = .740$$

Some atomic arrangements require description where repeating unit contains more than a single atom.

Most famous / simplest example is honeycomb (hexagonal) lattice



Suppose you tried to generate by using \hat{a}_1 and \hat{a}_2 shown.

Would not work because

$\hat{a}_1 + \hat{a}_2$ would give a point \times not occupied by an atom

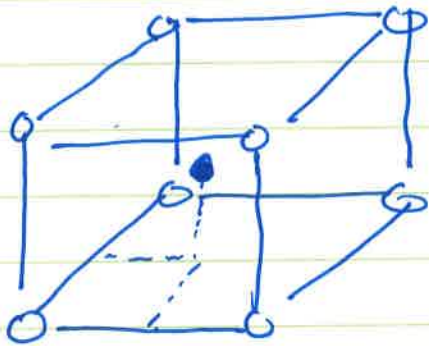
Instead, use \vec{a}_1, \vec{a}_2 repeating object is $\text{O} \text{---} \text{O}$ containing two atoms.

Can use a non primitive unit cell

(non minimal area/volume) and a basis eg

$$\text{bcc} \quad \left. \begin{array}{l} \hat{a}_1 = a\hat{x} \\ \hat{a}_2 = a\hat{y} \\ \hat{a}_3 = a\hat{z} \end{array} \right\} \text{volume} = a^3 > \frac{3}{4} a^3 \text{ previously}$$

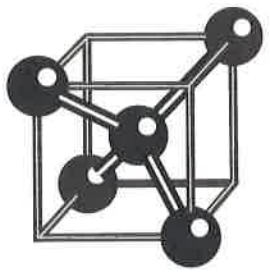
+ basis : atoms at $\vec{0}$ and $\frac{a}{2}(\hat{x} + \hat{y} + \hat{z})$



Popular Lattices

FCC with Basis

| | |
|--------------|------|
| c | 3.57 |
| Si | 5.43 |
| Ge | 5.66 |
| α -Sn | 6.49 |



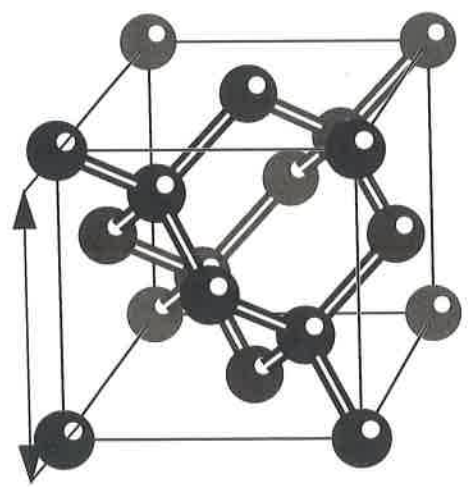
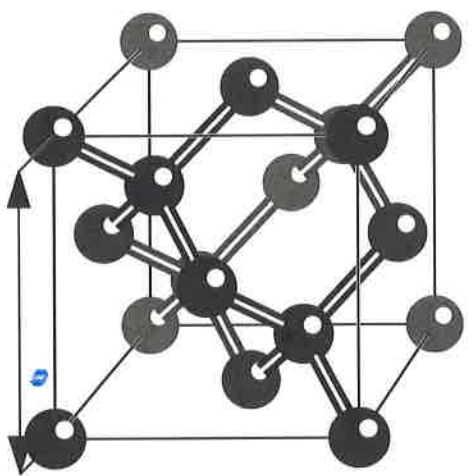
$$\vec{r} = \frac{a}{4} (\hat{x} + \hat{y} + \hat{z})$$

BOTH ATOMS SAME

Diamond

(4 elements)

less obvious, but like hexagonal a basis is required



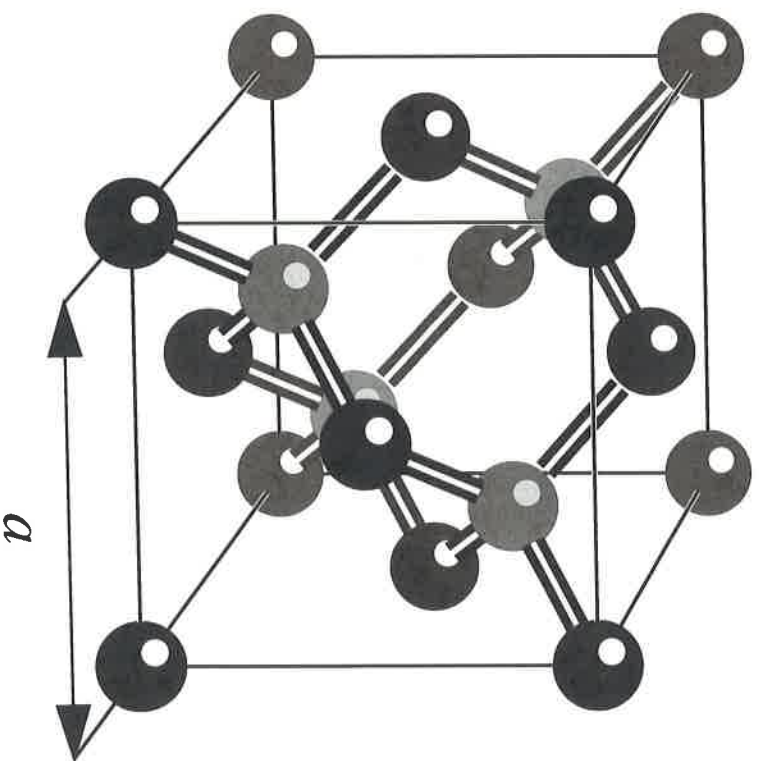
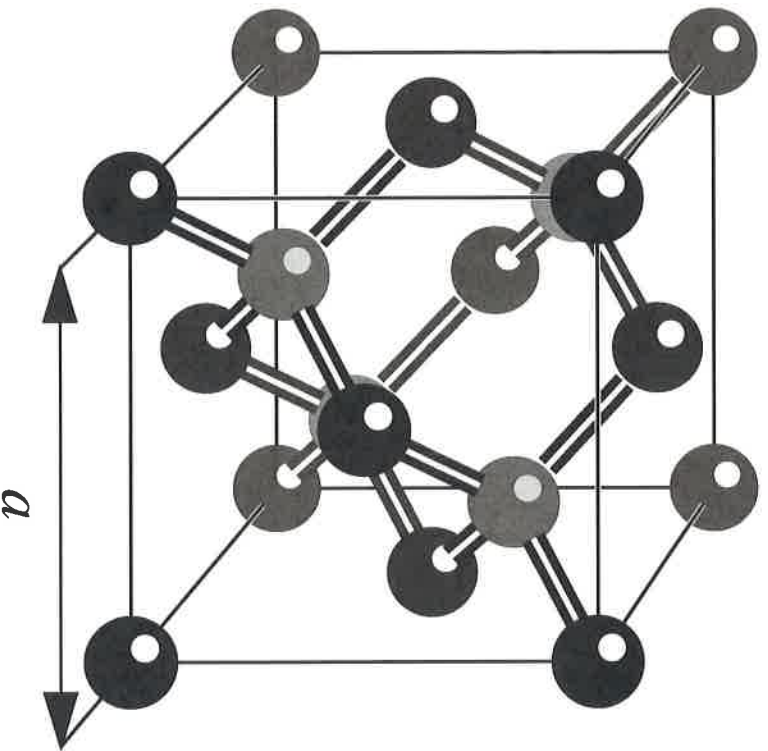
Popular Lattices

FCC WITH BASIS

TWO ATOMS DISTINCT

Zincblende

| | | | | |
|------|------|------|------|------|
| CuF | 5.26 | ZnS | 5.41 | AlSb |
| CuCl | 5.41 | InSe | 5.67 | Gap |
| CuBr | 5.69 | | | GapS |
| CuI | | | | GaSb |
| AgI | | | | InP |
| | | | | InAs |
| | | | | InSb |
| | | | | SiC |



~
doped
semiconductors
Si, Ge
not 1:1
but small
amount

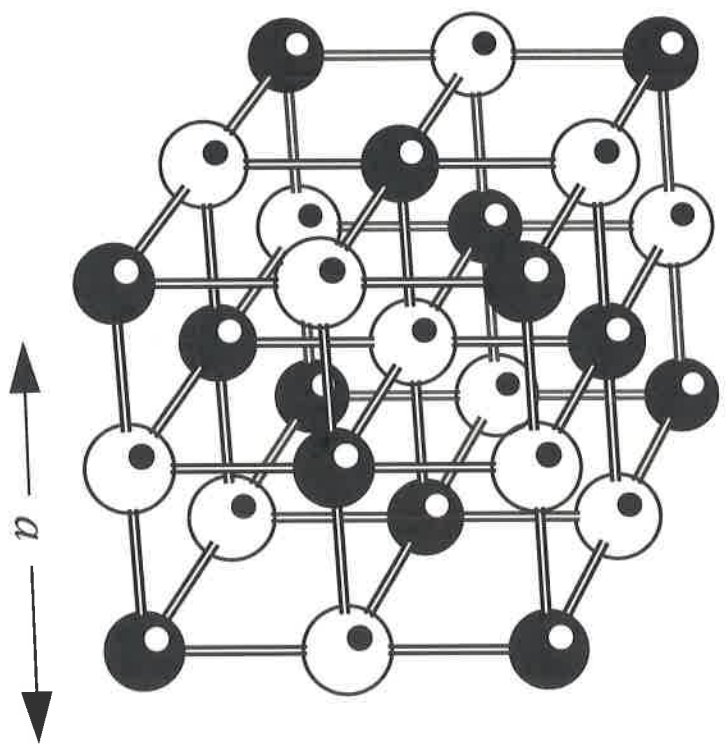
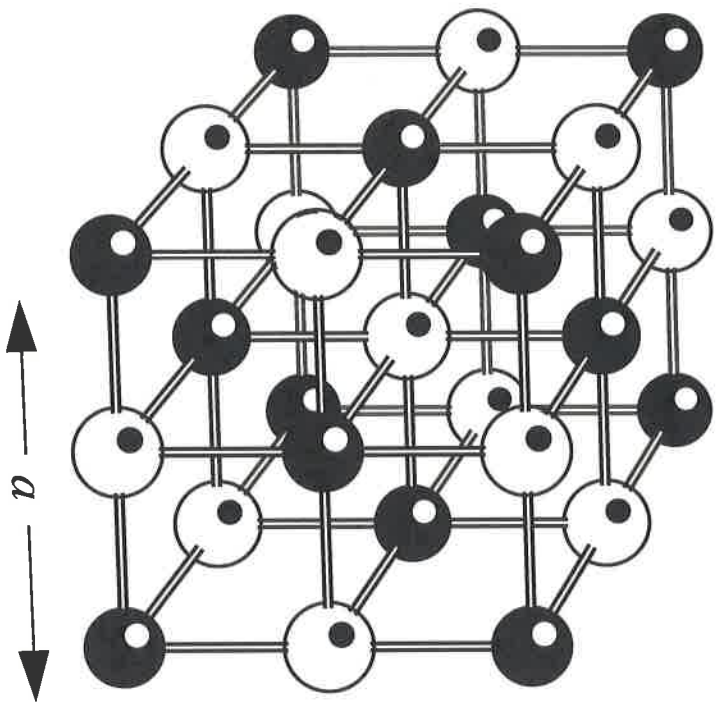
Popular Lattices

LiF
LiCl
LiBr
LiI
NaF
NaCl
NaBr
!

4.02
5.13
5.50
RbF
RbCl
CsF
CsCl

Two interpenetrating
fcc lattices

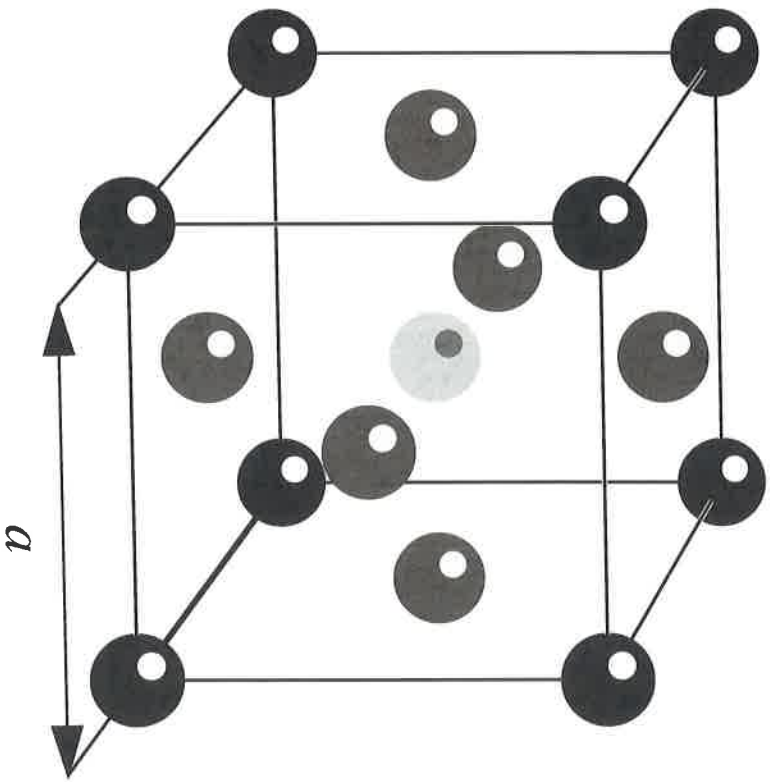
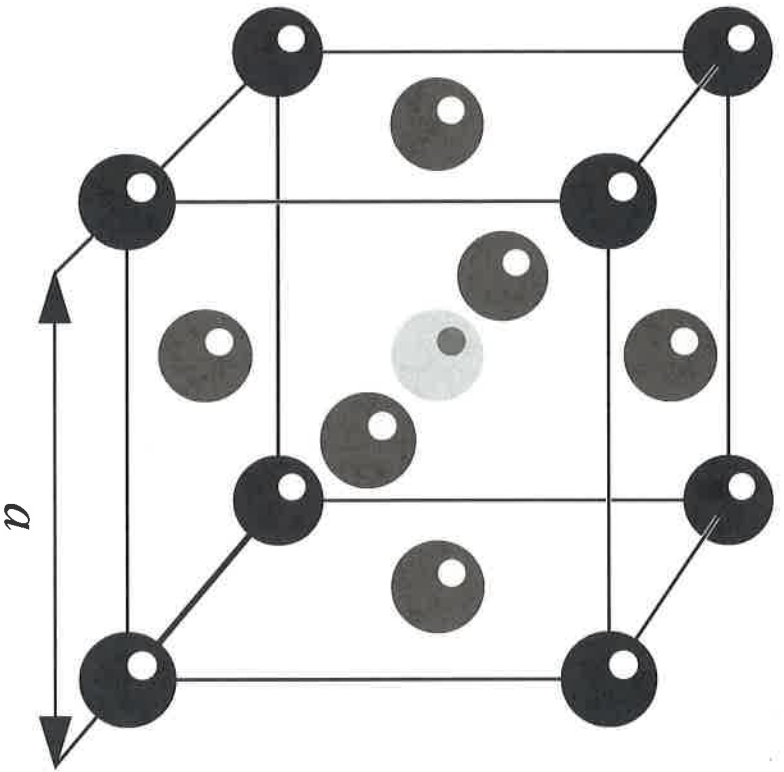
Sodium Chloride (NaCl)



Popular Lattices

113

Perovskite

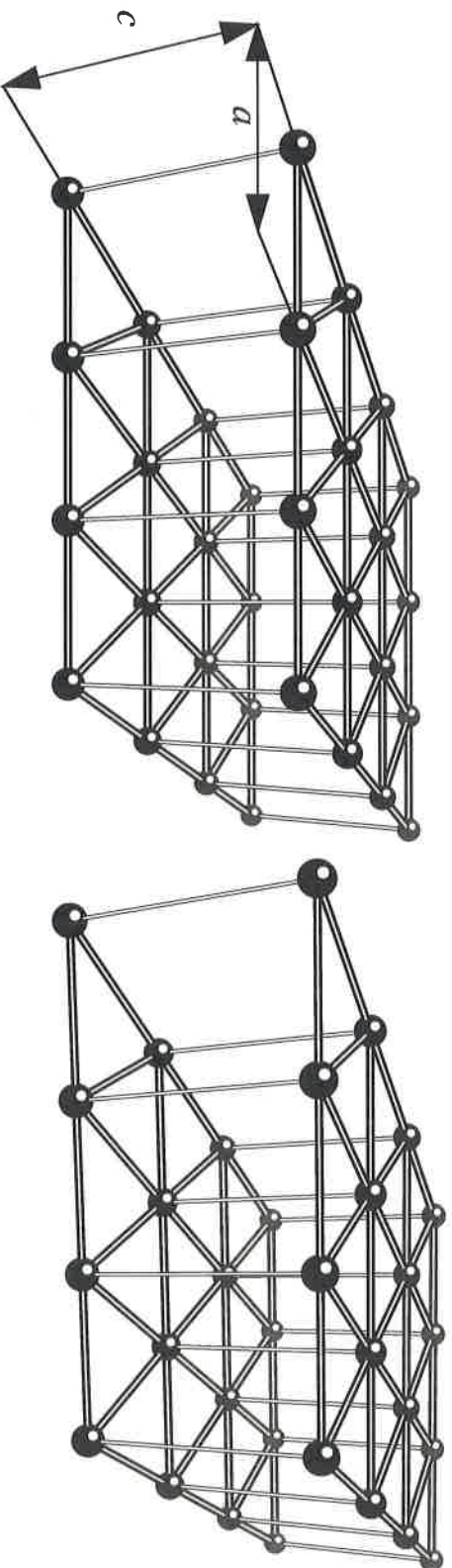


Popular Lattices

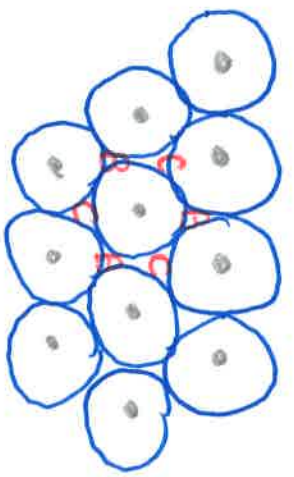
$$\begin{aligned}\hat{a}_1 &= a\hat{x} \\ \hat{a}_2 &= \frac{a}{2}\hat{x} + \frac{\sqrt{3}}{2}a\hat{y} \\ \hat{a}_3 &= c\hat{z}\end{aligned}$$

Hexagonal

Two triangular lattices
directly on top of each other



Popular Lattices

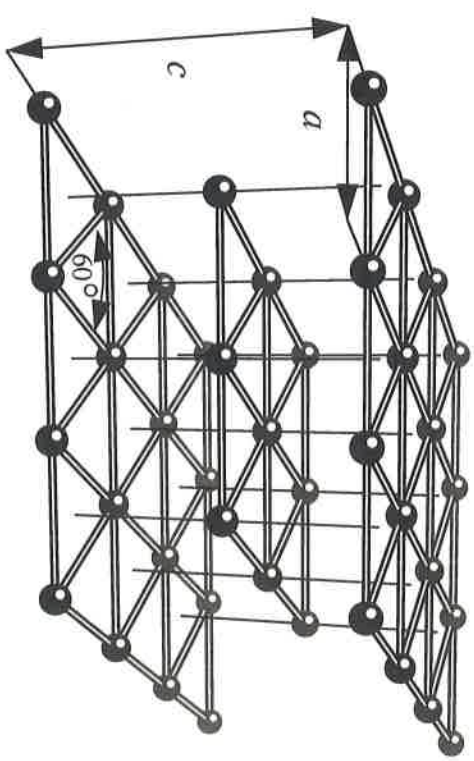
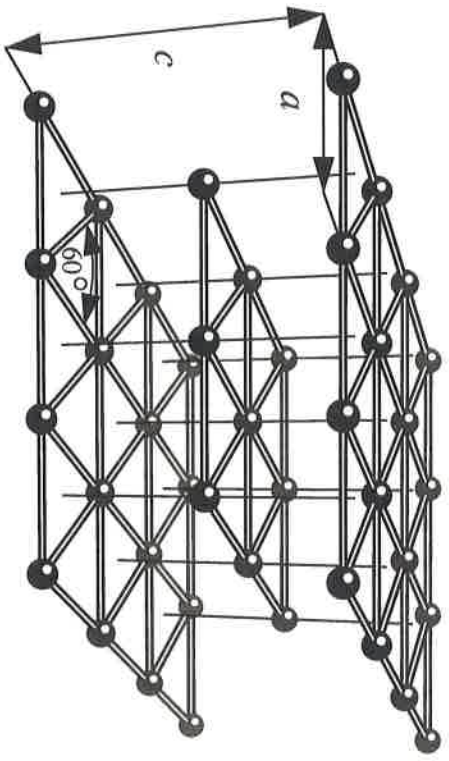


HCP IS
 ABABAB
 FCC IS
 ABCABC
 PUT BALLS
 AT INDENTATIONS
 ON PLANES BELOW

Hexagonal Close Packed (hcp)

30 elements!

| | a | c | c/a | hard spheres |
|------|------|------|------|--|
| BCC | 2.29 | 3.58 | 1.56 | $c = \sqrt{\frac{8}{3}} a$ $= 1.63299a$ |
| CD | 2.98 | 5.62 | 1.89 | |
| CE | 3.65 | 5.96 | 1.63 | |
| a-co | 2.51 | 4.07 | 1.62 | |

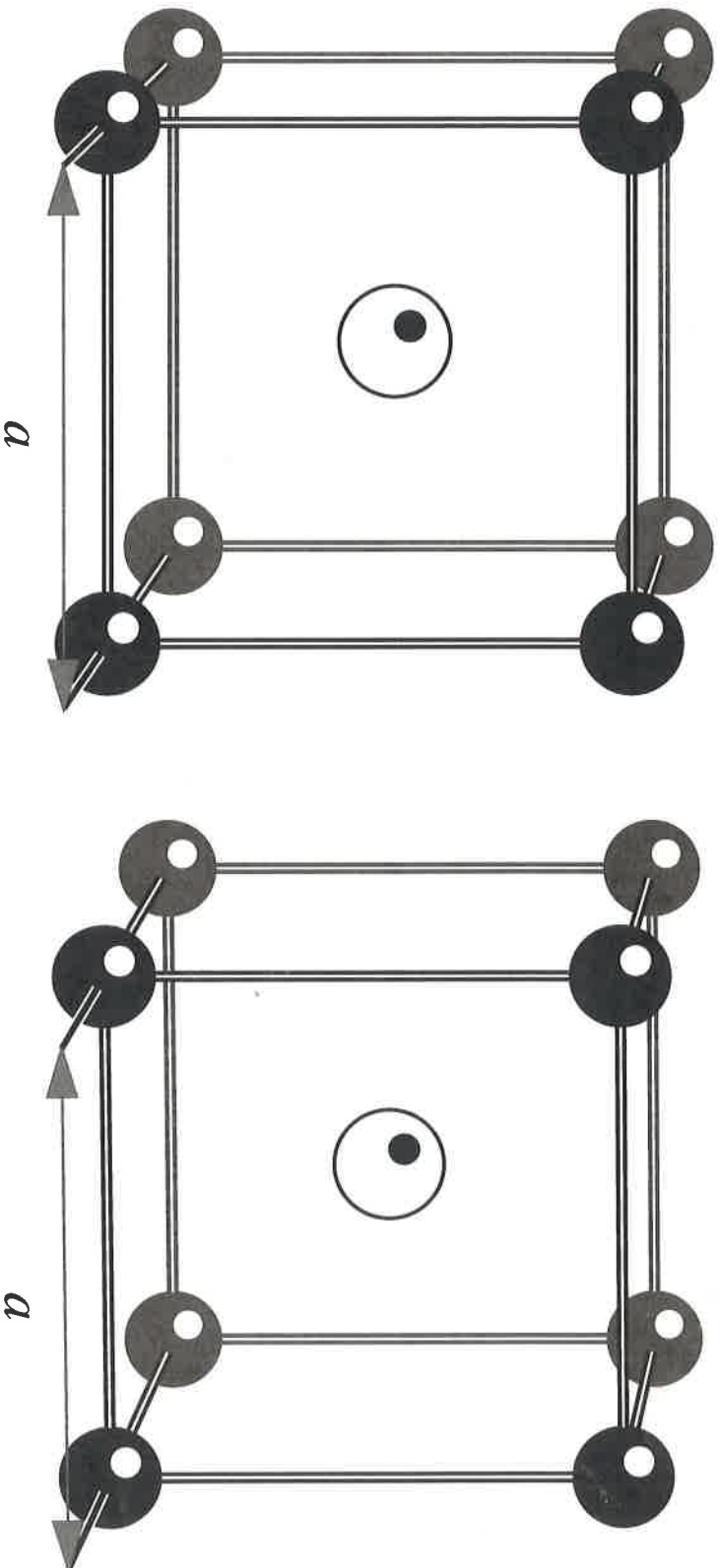


1

Popular Lattices

Cesium Chloride (CeCl)

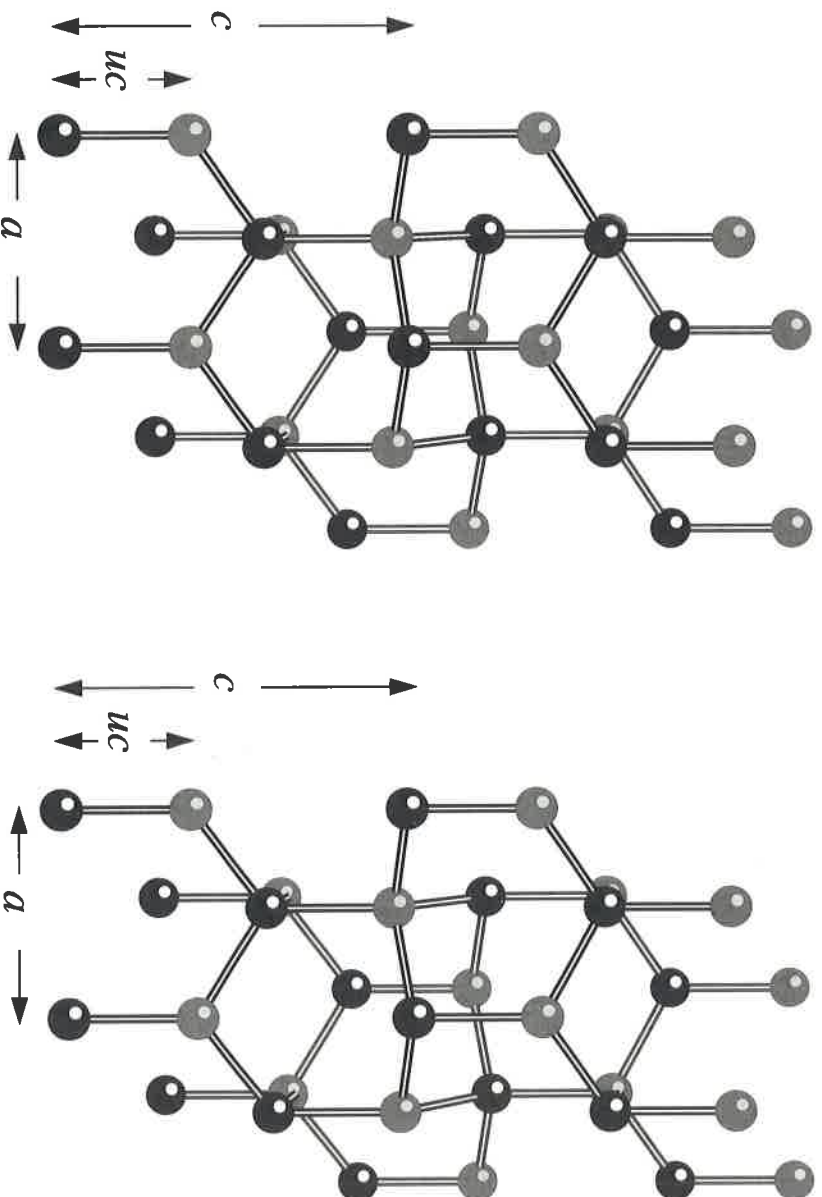
*BCC with
alternating
species*



Popular Lattices

SKIP

Wurtzite



See periodic tables in kit

project:

FCC/BCC/SC/EX

BCC and FCC examples (Elements)

| FCC | Ar | 5.26 | Ir | 3.84 | Pt |
|-----------------------------|-------------|------|----|------|---------|
| lattice constant in Å | Ag | 4.09 | Kr | | 8-Pu |
| | Al | 4.05 | La | | Rh |
| | Au | 4.08 | Ne | | Sc |
| | Ca | 5.58 | Ni | | Sr |
| | Ce | 5.16 | Pb | | Th |
| | β -Co | 3.55 | Pd | | Xe |
| | Cu | 3.61 | Pr | | Yb 5.49 |
| | | | | | |
| | | | | | |
| | | | | | |

| BCC | Ba | 5.02 | Li | Ta |
|-----|----|------|----|----|
| | Cr | 2.88 | Mo | Tl |
| | Cs | 6.05 | Na | V |
| | Fe | 2.87 | Nb | W |
| | K | 5.23 | Rb | |

SC is very rare (only one type of Po!)

Why do you think? (Too empty?)

project:

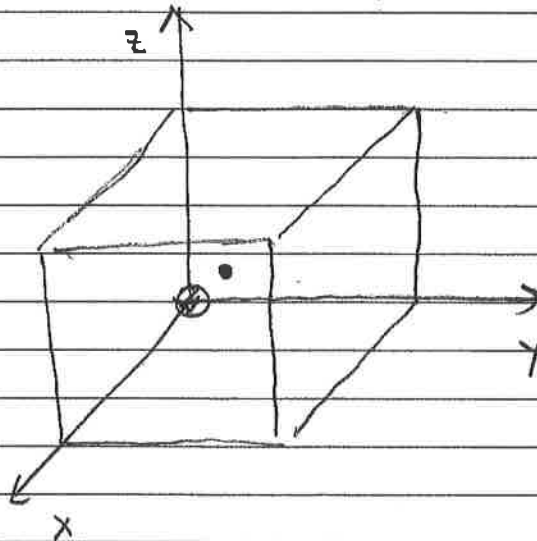
HCP-1

Diamond, Hexagonal Close packed, and NaCl

Diamond structure

FCC lattice with basis $\vec{0}, \frac{a}{4}(\hat{x} + \hat{y} + \hat{z})$

| | |
|--------------|------|
| C | 3.57 |
| Si | 5.43 |
| Ge | 5.66 |
| α -Sn | 6.49 |



Zincblende

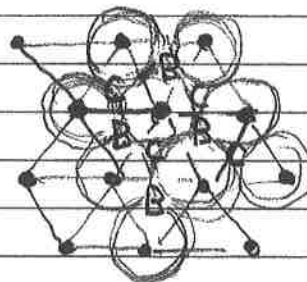
⊙ and • are different atoms

| | | | | | |
|------|------|------|------|------|------|
| CuF | 4.26 | ZnS | 5.41 | AlSb | 6.13 |
| CuCl | 5.41 | ZnSe | 5.67 | GaP | |
| CuBr | 5.69 | : | : | GaAs | |
| CuI | : | : | : | GaSb | |
| AgI | | | | InP | |
| BeS | | | | InAs | |
| BeSe | | | | InSb | |
| BeTe | | | | SiC | 4.35 |
| MnS | | | | | |
| MnSe | | AlAs | 5.62 | | |

doped semiconductors
Si:C
↑
not 1:1
but small amounts.

Hexagonal Close Packed

Plane:



next plane: balls lie at B indentations of 1st plane

Note two choices: could occupy C

DiVOGA

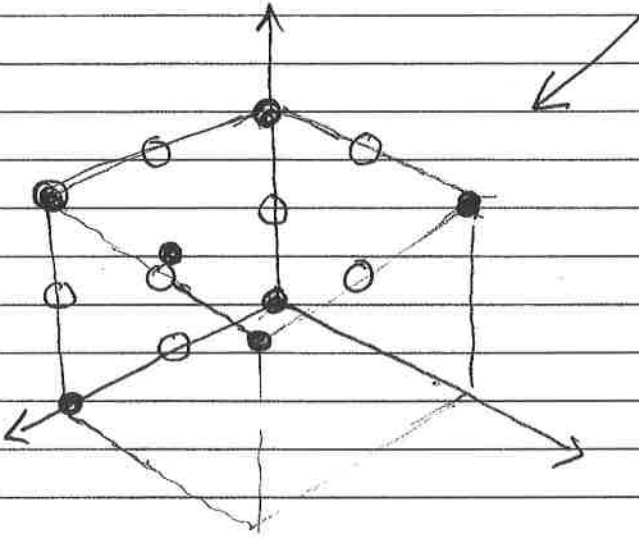
HCP is ABABAB } others uncommon
FCC is ABCABCABC

project:

HCP-2

NaCl structure

2 interpenetrating fcc lattices



| | | | | | |
|------|------|------|------|------|------|
| LiF | 4.02 | RbF | 5.64 | CaS | 5.69 |
| LiCl | 5.13 | RbCl | 6.58 | CaSe | 5.71 |
| LiBr | 5.50 | : | : | : | : |
| LiI | : | : | : | : | : |
| NaF | : | : | : | : | : |
| NaCl | : | : | : | : | : |
| NaBr | : | : | : | : | : |
| NaI | : | : | : | : | : |
| KF | : | : | : | : | : |
| KCl | : | : | : | : | : |
| KI | 7.07 | CaO | 4.81 | BaTe | 6.99 |

Many elements adopt multiple crystal structures between 0 K and their melting temperature. Plutonium has a particularly elaborate phase diagram:

| Transformation Temp, C | Phase | Structure (atoms per unit cell) | Density (g/cc) |
|------------------------|------------|---------------------------------|----------------|
| 112 | α | monoclinic (16) | 19.8 |
| 185 | β | fc monoclinic (34) | 17.8 |
| 310 | γ | fc orthorhombic (8) | 17.1 |
| 450 | δ | fcc (4) | 15.9 |
| 475 | δ' | fc tetragonal (2) | 16.0 |
| 640 | ϵ | bcc (2) | 16.5 |

Table 1: Source, Atomic Weapons Establishment, [Discovery Article](#)